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Quantum Transport with Band-Structure and Schottky Contacts

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We describe (i) a parameterized single band model that mimics the full-band , -valley non-parabolicity, (ii) a method for calculating the semi-classical and quantum electron charge with the sp3s* bandstructure model, and (iii) a Schottky contact model compatible with any localized orbital bandstructure model.
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For state-of-the-art In-based resonant tunneling diodes (RTDs) [1], transport takes place solely within the , valley of the conduction band. However, the non-parabolicity is so large that we are forced to use a 10-band sp3s* model [2]. Modeling transport in a single valley of a single band with a full 10-band model is inefficient. Therefore, we describe a parameterized 1-band tight-binding model that mimics the the full-band , -valley non-parabolicity. To make quantitative comparisons with experimental results, a self-consistent quantum charge calculation is also generally required. As part of that calculation, we describe our improved method for calculating the semi-classical and quantum electron charge, Fermi-level, and Jacobian that is consistent with the full bandstructure model. Finally, we describe our Schottky contact model that is compatible with any localized orbital bandstructure model.

To mimic the , -valley non-parabolicity with a single-band model, we parameterize as functions of kinetic energy and transverse momentum the hopping elements and site energies of the 1-band, tight-binding Hamiltonian according to

$$E_k = 2t(E_k, k_t)\left[1 - \cos k_z a\right] + D(E_k, k_t) \tag{1}$$

where E_k is the kinetic energy, k_t is the transverse (real) wavevector, k_z is the longitudinal (in general complex) wavevector, t is the hopping element, and D is the correction to the site energy. The arrays $t(E_k, k_t)$ and $D(E_k, k_t)$ are created from the bulk $\epsilon(\mathbf{k})$ dispersion relation and then used for interpolation in the transport calculation.

The arrays are created from the following algorithm. For each k_t, the kinetic energy, E_k, is swept from a minimum to maximum value. At each E_k value, k_z is found from the full-band dispersion relation, $\epsilon(\mathbf{k})$. Near the conduction band edge, $t(E_k, k_t)$ is found from $t(E_k, k_t) = \partial^2 E_k/\partial k_z^2 \left[2a^2 cos k_z a\right]^{-1}$ where the derivative is obtained from $\epsilon(\mathbf{k})$. At higher energies, the dispersion becomes fairly linear and we find $t(E_k, k_t)$ from the first derivative: $t(E_k, k_t) = \partial E_k/\partial k_z \left[2a \sin k_z a\right]^{-1}$. Thus, we choose t to give the correct effective mass or group velocity. With t set, we then choose D to give the correct energy, i.e. $D(E_k, k_t) = E_k - 2t(E_k, k_t)\left[1 - \cos k_z a\right]$. At each point of the actual dispersion we are choosing a tight-binding dispersion with the correct slope or curvature. We then add a site potential to move the tight-binding dispersion up or down to get the right energy.

For the transport calculations, we work with total energy, E, and transverse momentum, k_t [3]. Foreach E, k_t and site i, we calculate the kinetic energy, $E_k = E - V_i$, and then interpolate from $D(E_k, k_t)$ and $t(E_k, k_t)$ to obtain the Hamiltonian elements, $D_i(E, k_t)$ and $t_{i,i\pm1}(E, k_t)$. The averaged value of t is used between sites, and the site energy at site i is given by $t^- + t^+ + V_i + D_i$ where $t^{\pm} = (t_i + t_{i\pm1})/2$. This reproduces the standard tight-binding Hamiltonian for a cosine dispersion.

Generally, in modeling a semiconductor device, a contact doping is specified from which the contact Fermi level is calculated. If the contact Fermi level is not calculated using the same band-structure model as that used for the transport calculations, the quantum-charge calculation in the device will be incorrect. We describe our method for calculating the semiclassical Fermi-level, charge, and Jacobian using the bandstructure generated from the Hamiltonian. Then we describe our quantum Jacobian for calculating the quantum charge.

We begin with the general expression for the electron density since our contact Hamiltonian contains a small imaginary potential which creates small band-tails, alters the density of states, and thus slightly alters the Fermi-level [3].

$$n = \int_{-\infty}^{\infty} \frac{dE}{2\pi} A(E) f(E - E_f) \tag{2}$$

where the spectral function is given by (assuming spin degeneracy)

$$A(E) \;=\; \int \frac{d^3k}{4\pi^3} \frac{\eta(E)}{\left(E-\epsilon(\mathbf{k})\right)^2+\eta^2(E)} \tag{3}$$

$f(E-E_f)$ is the Fermi factor, $\epsilon(\mathbf{k})$ is the dispersion relation generated from the Hamiltonian, $H(\mathbf{k})$, and $\eta(E)$ is the energy-dependent broadening factor from the imaginary potential [3]. For a spherically symmetric dispersion centered at the , valley, Eqs. (2) and (3) become

$$n \;=\; \frac{1}{\pi^3}\int_0^{k_{max}} dk k^2 \int_{-\infty}^{\infty} dE \frac{f(E-E_f)\,\eta(E)}{\left(E-\epsilon(k)\right)^2+\eta^2(E)} \tag{4}$$

The order of integration is chosen for numerical efficiency. $f(E-E_f)$ varies rapidly only around E_f and the spectral function is peaked at $E=\epsilon(k)$. Relatively few k points can be used and the energy points are chosen to resolve the regions around E_f and $\epsilon(k)$. The Newton-Raphson scheme for calculating the self-consistent electrostatic potential requires an expression for $\partial n/\partial\phi$ where ϕ is the electrostatic potential. We use the approximation

$$\partial n/\partial\phi \approx q\partial n/\partial E_f \tag{5}$$

which is exact in the absence of broadening.

In the absence of broadening, the spectral function is a delta function and Eq. (4) becomes

$$n \;=\; \frac{1}{\pi^2}\int_0^{k_{max}} dk k^2 f(\epsilon(k)-E_f) \tag{6}$$

Integrating by parts and substituting variables $E=\epsilon(k)$, Eq. (6) becomes

$$n \;=\; \frac{1}{3\pi^2}\int_{E(k=0)}^{E(k_{max})} dE k^3(E) \frac{-\partial f(E-E_f)}{\partial E} \tag{7}$$

In Eq. (7), $k^3(E)$ is the inverse of the dispersion relation $\epsilon(k)$ raised to the third power valid if the dispersion is single-valued within the domain of integration. We cast Eq. (6) in the form of Eq. (7) for numerical efficiency. The integrand is only rapidly varying around E_f, so that it is straightforward to integrate for any temperature. For the Jacobian, we take $\partial/\partial E_f$ of Eq. (7).

So far, we have discussed the semi-classical calculation of the Fermi-level, charge, and Jacobian using realistic bandstructure. We must also calculate the quantum charge and a corresponding Jacobian. We have been using the the semiclassical Jacobian for the quantum calculation [3], but it is more efficient and even easier to compute an approximation for the quantum Jacobian. In the equilibrium region of the leads, using approximation (5), $\partial n/\partial\phi$ is given by

$$\frac{\partial n}{\partial\phi} = \frac{2q}{a}\int\frac{d^2k_t}{4\pi^2}\int\frac{dE}{2\pi}\,\frac{-\partial f(E-E_f)}{\partial E}\mathrm{tr}\left\{A_{L,L}(\mathbf{k_t},E)\right\} \tag{8}$$

where $A_{L,L}(\mathbf{k_t},E)$ is the spectral function at layer L, $\mathbf{k_t}$ is the transverse wavevector, a is the layer thickness, and the trace is over the cation and anion orbitals.

In the non-equilibrium region, in the absence of incoherent scattering, the expression for the electron density has two components resulting from injection from the left and right contacts [3]. Using approximation (5) on each component, we obtain

$$\frac{\partial n}{\partial\phi} = \frac{2q}{a}\int\frac{dE}{2\pi}\int\frac{d^2k}{4\pi^2}\left[\frac{-\partial f(E-E_f^{\mathcal{L}})}{\partial E}\mathrm{tr}\left\{A_{L,L}^{\mathcal{L}}(\mathbf{k},E)\right\} \;+\; \frac{-\partial f(E-E_f^{\mathcal{R}})}{\partial E}\mathrm{tr}\left\{A_{L,L}^{\mathcal{R}}(\mathbf{k},E)\right\}\right] \tag{9}$$

where $A_{L,L}^{\mathcal{L}} = G_{L,1}^R\,{}^{B\mathcal{L}}_{1,1}G_{1,L}^A$ and , $^{B\mathcal{L}}$ is the anti-Hermitian component of the left boundary self-energy [3]. Eqs. (8) and (9) are calculated in the same loop as the quantum charge making the calculation very efficient. Even in the presence of incoherent scattering, the expression for $G^<$ can be broken up into components contributed from the left and right contacts; however, seperating the components increases the computational burden of the scattering calculation by a factor of two.

Modeling the effect of Schottky contacts requires a model for the metal that is compatible with the localized orbital bandstructure model for the semiconductor. The microscopic physics of the semiconductor - metal interface is complex. The electrical characteristics of the standard model [4] depend on the presence of an interfacial layer of atomic

dimensions. Rather than attempt a microscopic model of the interface, we present a model which reproduces the essential macroscopic electric properties of the interface. The metal layer enters Poisson's equation and Schrödinger's equation as a boundary condition on the semiconductor region.

For Poisson's equation, the metal is an equipotential region with a Fermi-level fixed by the applied potential. The Fermi-level of the metal is assumed to be pinned relative to the valence band of the semiconductor. The metal fixes the electrostatic potential of the adjacent semiconductor atomic layer resulting in a Dirichlet boundary condition on Poisson's equation. A metal also gives rise to an image potential which is added to the electrostatic potential of the semiconductor:

$$V(z) = \sum_{i=\mathcal{L}/\mathcal{R}} \frac{-q^2}{16\pi\epsilon|z - z_i|} \tag{10}$$

where $z_{\mathcal{L}/\mathcal{R}}$ is the position of the left/right metal - semiconductor interface defined as $a/2$ to the left of the first semiconductor layer and $a/2$ to the right of the last semiconductor layer, respectively.

For Schrödinger's equation, the metal region acts as a source and sink of electrons for the semiconductor. Since we do not know a priori into which semiconductor bands and from which semiconductor bands electrons will be sourced or sunk, we create a boundary self-energy which allows sourcing and sinking of electrons from all semiconductor bands. A general form of the boundary self energy is given by $-t_{1,0}\chi Z\chi^{-1}$ where $t_{1,0}$ is the block matrix coupling the device to the left lead, χ is the matrix of Bloch states, and Z is the diagonal matrix of propagation factors [3]. For a given energy and momentum, most of the bands will be evanescent resulting in propagation factors $z_j = e^{ik_j a}$ for which k_j is complex with a large imaginary component. To allow electrons to be absorbed by the metal contacts from any semiconductor band, we set the elements of the matrix of propagation factors to be $z_j = i\eta$ independent of energy and momentum. Since Z is now a constant times the identity matrix, the boundary self energy becomes

$$\Sigma_{1,1}^{RB} \;=\; -i\eta t_{1,0} \tag{11}$$

To obtain an estimate for the magnitude of η, we consider a metal Fermi level around mid-band with $k = \pi/2a$ resulting in a propagation factor $e^{ika} = i$ which gives a value for η of 1 and a boundary self energy of $\Sigma_{1,1}^{RB} = -it_{1,0}$.

In summary, we have presented several improvements and enhancements of the charge models, bandstructure models, and contact models described in [3] which increase the comprehensiveness and numerical efficiency of our approach.

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